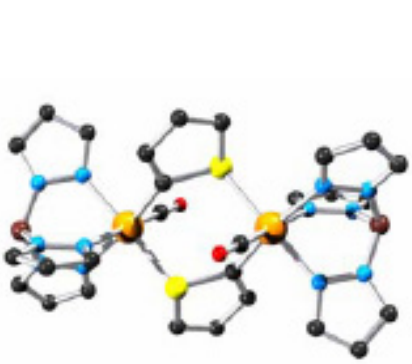
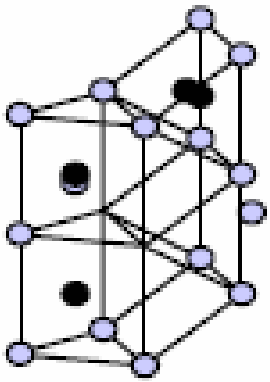
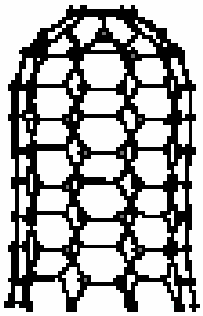
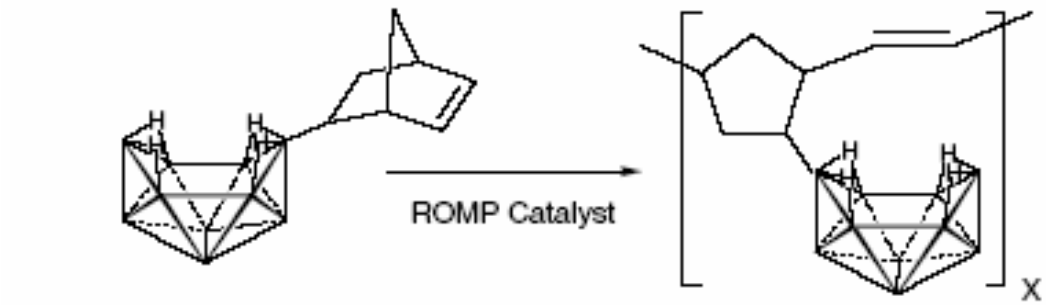
Frontiers in

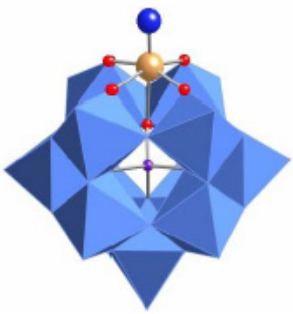
CATALYSIS SCIENCE

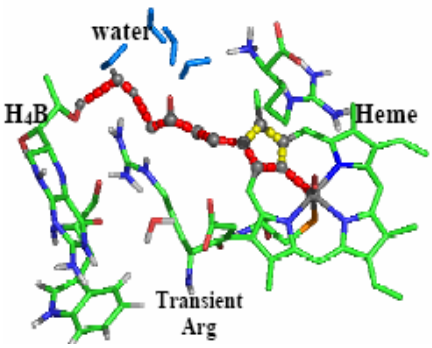


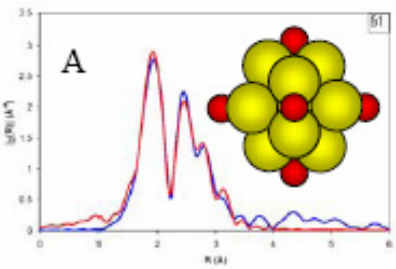












Meeting of the Catalysis and Chemical Transformations Program

Chemical Sciences, Geosciences and Biosciences Division

Office of Basic Energy Sciences, U.S. Department of Energy

Rockville, MD **May 23-26, 2004**

This document was produced under contract number DE-AC05-00OR22750 between the U.S. Department of Energy and Oak Ridge Associated Universities.

FOREWORD

This meeting of the Catalysis and Chemical Transformations Program is sponsored by the Division of Chemical Sciences, Geosciences and Biosciences, Office of Basic Energy Sciences (OBES), U.S. Department of Energy. It is being held on May 23-26, 2004, at the Doubletree Hotel, Rockville, MD.

The purposes of this meeting are three-fold:

- to give participants an appreciation of the broad range of research topics currently supported by our program under the umbrella of catalysis and related sciences;
- to foster exchange of ideas and cooperation among participants;
- to discuss the exciting new opportunities for catalysis science, both at its core and at its interfaces with other disciplines, including materials science, biosciences, theory and simulation, instrumentation and analytical science.

Catalysis activities within OBES emphasize fundamental research aimed at understanding and controlling the chemical reactivity of fluid and condensed matter. The long-term goal of this research is to discover the natural laws and generalizations that enable the prediction of structure-reactivity relations. Such knowledge, together with our ability to synthesize complex structures, will help us to guide chemical reactions along desired pathways. Ultimately, these fundamental concepts will help promote efficient conversion of natural and synthetic resources, with minimum impact to our environment.

Special thanks go to our guest keynote speakers, who will expose us to recent advances in fields that lie both at the core of catalysis and at its boundaries with other multidisciplinary fields. The poster sessions have been designed to allow everyone to present their recent scientific outcomes, and to share ideas and opinions. The breakout sessions will permit participants to discuss the future prospects for these lively sciences.

The breakout aspect of this meeting was kindly organized by Drs. Bob Bergman, John Bercaw, Tom Rauchfuss, Dave Dixon, Eric McFarland, Daniel Resasco, Juergen Eckert and Miquel Salmeron, and we deeply appreciate their tremendous effort. We also thank the Oak Ridge Institute of Science and Education staff, Ms. Julie Malicoat in particular, for the logistical support and the compilation of this volume. We are indebted to the program participants, as you have worked hard to produce oral and poster presentations; to the session moderators, and to the rest of attendees, for their contributions.

Have a productive, highly interactive, and stimulating meeting.

John Gordon and Raul Miranda
Chemical Sciences, Geosciences and Biosciences Division
U.S. DOE – BES

This page intentionally left blank.

Table of Contents

Table of Contents

Meeting Agenda

2004 Catalysis Contractors' Workshop

Rockville, MD
May 23-26, 2004
(by invitation only)

Tentative Agenda

Day 1: May 23, 2004

5:00 p.m. Regency Room open and available for poster setup

Approximately
6:00 p.m. Dinner

Session A. **Posters I** (numbers 1-60)

8:00-10:00 p.m. **Poster Opening Session**

Day 2: May 24, 2004

8:00 a.m. COFFEE

8:30 **Workshop Overview**

Session B. **Focus on Materials**
Moderator: **Tom Rauchfuss**

9:00-10.00 **Invited Speaker- FRAZER STODDART (UCLA)**

10:00-10:20 COFFEE

10:20-10.40 **Larry Sita** (U. Maryland, College Park)

10:40-11:00 **Jeff Long** (UC Berkeley)

11:00-11:20 **Jeff Brinker** (Sandia N.L. – U. New Mexico)

11:20-11:40 **Larry Scott** (Boston College)

11:40-12.00 Discussion

12:00 LUNCH
CCT Performance

Session C. **Focus on Heterogeneous Catalysis and Surface Chemistry**
Moderator: **Jan Hrbek**

1:30-2:30	**INVITED Speaker- ROBERT SCHLÖGL (Fritz-Haber Institut)** ***The Impact of In-situ Analysis of Heterogeneous Catalysts for the Improvement of Their Function***
2:30 -2:50	COFFEE
2:50-3:10	**Jim Dumesic** (Wisconsin)
3:10-3:30	**Eric Altman** (Yale)
3:30-3:50	**Jose Rodriguez** (BNL)
3:50-4:10	**Chris Jones** (Georgia Tech)
4:10-4:30	Discussion
4:30-6:00	Poster exchange: take down numbers 1-60; put up numbers 61-120
6:00	Dinner
	INVITED Speaker – MICHELLE BUCHANAN (Oak Ridge National Laboratory) *The Hydrogen Economy: Opportunities for Fundamental Research to Address some Grand Challenges*
8:00-10:00 p.m.	Session A. **Posters II** (numbers 61-120)

<u>Day 3: May 25, 2004</u>

8:00 a.m.	COFFEE

Session D. **Focus on Homogeneous Catalysis**
Moderator: **John Bercaw**

8:30-9:30	**INVITED Speaker- GEOFF COATES (Cornell University)** *Discovery, Development, and Application of Catalysts for the Synthesis of Defined Polymer Architectures*
9:30-9:50	**Ged Parkin** (Columbia)
9:50-10:10	**John Hartwig** (Yale)
10:10-10:30	**Susannah Scott** (UC Santa Barbara)

10:30-10:50 Discussion

10.50-11:00 COFFEE

Session E. **Focus on Biocatalysis**
Moderator : **Ged Parkin**

11:00-11:20 **Matt Kanan and David Liu (Harvard) – Invited Short Presentation**
A New Approach to the Discovery of Bond Forming Chemical Reactions

11:20-11:40 **Larry Que** (Minnesota)

11:40-12:00 Discussion

12:00-12:50 LUNCH

12:50-1:50 **INVITED Speaker- HOWARD TURNER (SYMYX)**

2:00-5:30 Breakout Sessions

Moderators: **Bob Bergman, John Bercaw, Dave Dixon, Dan Resasco, Eric McFarland, Tom Rauchfuss**, **Miguel Salmeron, Juergen Eckert**

6:00 Posters down

6:30 DINNER

INVITED Speaker – RICHARD CATLOW (University College London)
Computer Modelling as a Tool in Catalytic Science

8:00 Evening free to general participants. Moderators write up conclusions and recommendations.

Day 4: May 26, 2004

8:00 a.m.	COFFEE

Session F. **Focus on Instrumentation, Theory and Simulation**
Moderator: **Dave Dixon**

8:30-8:50	**Mike Deem** (Rice University)
8:50-9:10	**Manos Mavrikakis** (U. Wisconsin)
9:10-9:30	**Miquel Salmeron** (L. Berkeley National Lab.)
9:30-9:50	**Ralph Nuzzo** (U. Illinois)
9:50-10:10	Discussion
10:10-10:30	COFFEE
10:30	Summary and Discussion from Breakouts A-D
12:00	Working Lunch
	Conclusions
	Recommendations for Future Workshops
2:00	End of Meeting